REMARKS

Claims 1, 9, and 13-35 were pending. All claims were rejected for the reasons set forth in more detail below. We have amended claims 1, 9, and 13-35. No claims have been cancelled, added or withdrawn in the present Amendment. Claims 1, 9, and 13-35 remain pending. We respectfully request reconsideration.

As addressed in more detail below, we include herewith the Rule 132 Declaration of Dr. Christoph Steinbeck (herein Declaration). CambridgeSoft, the assignee of the above-identified application, has made available to Dr. Steinbeck a license to any patent issuing from the above-identified application for use in his open source development efforts.

Telephonic interviews of July 1, 2010, and August 3, 2010

We thank Examiner Jones for the telephonic interviews of July 1, 2010, and August 3, 2010, with the undersigned. During the interview, the participants discussed claims 1 and 26-27 and Helson, "Simulation of Carbene Chemistry and Other Problems in Computer-Assisted Organic Synthesis", Purdue University 1993 (herein Helson) and Benecke, C., *et al.* and "MOLGEN+, a generator of connectivity isomers and stereoisomers for molecular structure elucidation", *Analytica Chimica Acta*, Vol. 314, pp. 141-147, 1995 (herein Benecke). The participants also discussed the Examiner's concerns regarding the clarity of the steps recited in the claims as well as portions of the specification cited in the Office Action dated May 25, 2010. See Office Action at pg. 9.

No agreement was reached regarding the allowability of any claims. However, Examiner Jones was receptive to amendments proposed during the interviews.

Rejections under 35 U.S.C. § 103(a)

Claims 1, 9, and 13-35 were rejected under 35 U.S.C. § 103(a) as being obvious over Helson in view of Benecke. See Office Action at pg. 3. Specifically, the Office Action states that Helson teaches indentifying an instance of chemical structural symmetry and positioning atoms and bonds

in a chemical structure diagram. See Office Action at pgs. 3-4. The Office Action also states, however, that Helson does not disclose laying out atoms/bonds to express an identified symmetry. The Office Action relies on Benecke to provide this missing element, stating that Benecke "discloses laying out atoms/bonds to express the identified symmetry". See Office action at pg. 7.

Furthermore, the Office Action states that, "*Laying out the symmetrically equivalent atoms and bonds* by itself means that the symmetries are expressed. The claims do not require that the results be aesthetically pleasing." See Office Action at pg. 10 (emphasis in the original).

We have amended independent claims 1, 9, 28, and 35 and respectfully request reconsideration. The remarks that follow concern claim 1. However, claims 9, 28, and 35 include analogous limitations.

We have amended claim 1 to now require determining an arrangement of chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of the identified chemical structural symmetry in the chemical structure diagram. Further, the method of claim 1 also recites laying out the chemically symmetrically equivalent atoms and bonds in the chemical structure diagram in a two-dimensional pictorial representation of the chemical structure in accordance with the determined arrangement. In other words, claim 1 requires a purposeful determination of an arrangement of atoms and bonds to provide a **visually symmetric expression** of *chemical structural symmetry*.

We respectfully submit that none of the cited references teach or suggest making this determination, as explained in greater detail below. Thus, as the cited references do not teach or suggest all of the elements recited in amended claim 1, we also submit that claim 1 is patentable over the cited references.

Perception of Stereochemistry Does Not Determine Atom or Bond Arrangement

In our Amendment filed on March 2, 2010, we provided remarks in an attempt to clarify the relationship between the perception of stereochemistry and the process of structure diagram generation. These remarks remain relevant to the presently amended claims because the new limitation of "determining an arrangement of the chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of the identified chemical structural symmetry in the chemical structure diagram" falls squarely within the process of structure diagram generation. We restate our previous remarks in the context of our new amendment.

Stereochemical perception is a distinct and separate task from structure diagram generation, the later of which includes the determination of an arrangement of atoms and bonds to provide a visual expression of a chemical structure. Stereochemical perception is the process of identifying the relative spatial arrangement of atoms within molecules. Stereochemical perception is not concerned with the visual presentation of a molecular structure. Meanwhile, structure diagram generation is the process by which a two-dimensional arrangement of atoms and bonds in a molecule is determined from a connection table to provide a two-dimensional depiction of the chemical structure that can be displayed or printed.

In a stereochemical perception process, symmetry is consulted to determine if stereochemistry exists at an atom or bond. For example, if two substituents are symmetrically equivalent, then stereochemistry is said not to exist because a mirror image would be identical to the original. Also, when seeking to generate all molecular graphs that correspond to a given chemical formula, symmetry can be used to eliminate redundancies in the results. However, none of these considerations of symmetry have anything to do with determining an arrangement of atoms and bonds to provide a visual expression of a chemical structure corresponding to a given chemical formula.

Neither Helson, nor Benecke, alone or in combination, teach or suggest determining an arrangement of chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of identified chemical structural symmetry in a chemical structure diagram.

As mentioned above, the Examiner states that Helson does not disclose laying out atoms/bonds to express an identified symmetry. We agree. However, the Examiner also states, "*Laying out the symmetrically equivalent atoms and bonds* by itself means that the symmetries are expressed. The claims do not require that the results be aesthetically pleasing." See Office Action at pg. 10.

While we disagree that laying out atoms and bonds alone is the equivalent of laying out atoms and bonds to visually express an identified symmetry in light of the meaning given to those terms in the specification, we have amended claim 1 to avoid unintended interpretations. Specifically, claim 1 now recites determining an arrangement of chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of an identified chemical structural symmetry and laying out the chemically symmetrically equivalent atoms and bonds in a two-dimensional pictorial representation of the chemical structure in accordance with the determined arrangement.

Thus, we are not claiming merely displaying a representation of atoms and bonds of a chemical structure, which happens to possess an instance of chemical structural symmetry. Rather, claim 1 requires that the chemically symmetrically equivalent atoms and bonds be laid out in accordance with an arrangement that has been determined to provide a visually symmetric expression of an identified chemical structural symmetry. None of the cited references, alone or in combination, teach or suggest this combination of elements.

As mentioned above, the Office Action admits that Helson does not disclose symmetry as a consideration in laying out atoms and bonds in a pictorial representation of a chemical structure. Thus, we submit that Helson clearly does not teach or suggest determining an arrangement of chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of an identified chemical structural symmetry and laying out the chemically symmetrically equivalent atoms and bonds in a two-dimensional pictorial representation of the chemical structure

in accordance with the determined arrangement. So, too, does Benecke fail to provide these missing elements.

As described in detail in our previous responses, Benecke describes a structure generator software application, MOLGEN+, which produces all of the molecular graphs that correspond to a given chemical formula. As disclosed in Benecke, MOLGEN+ takes as its input a chemical formula, (optionally) prescribed and forbidden substructures, an interval for allowed ring sizes, and maximal bond multiplicities. From this input, MOLGEN+ generates a complete list of all mathematically possible molecular graphs that are compatible with the chemical formula. After generation of the constitutional isomers, MOLGEN+ produces a sketch of the molecules in the form of a tapestry of several molecules shown together or as a single molecule. See Benecke at pg. 142-44.

However, Benecke does not disclose determining an arrangement of chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of an identified chemical structural symmetry, as recited in amended claim 1. Benecke does mention symmetry, but only in the context of stereochemical perception. Specifically, Benecke uses chemical structural symmetry to eliminate redundancies in molecular graphs that would otherwise occur if chemical structural symmetry were not taken into account when generating all possible molecular graphs that correspond to a given chemical formula. Benecke's use of chemical structural symmetry has nothing to do with the visual presentation of a molecular structure.

Thus, when Benecke states, "MOLGEN+ is capable of generating all possible configurational isomers, again redundancy free (which also implies the consideration of symmetries)," Benecke is describing the use of chemical structural symmetry to remove an entire configurational isomer from the set of isomers that can eventually be displayed. See Benecke at pg. 145. This statement has nothing to do with the two-dimensional positioning of atoms and bonds in a pictorial representation of a chemical structure. The actual positioning of atoms and bonds in two-dimensions is a separate phase of the entire process.

Benecke does briefly address the phase of positioning atoms and bonds in two-dimensions for the purpose of providing a pictorial representation of possible chemical structures corresponding to a chemical formula. Specifically, Benecke states, "After generation of the constitutional isomers, you get a sketch of the molecules using a method based on [4]," (where [4] is a citation to a reference by C.A. Shelly). See Benecke at pg. 4. However, Benecke provides no details as to the actual process of determining the arrangement of atoms and bonds in such a sketch.

Benecke goes on to discuss techniques for computation of a placement of constitutional isomers in space (*i.e.*, in three dimensions). Specifically, Benecke states, "In the second step spatial realizations of these isomers are calculated by the application of appropriate geometrical transformations to the placement computed above." As to the details of these transformations, Benecke refers the reader to other references (specifically, references [7] and [8]) and provides no details as to the exact nature of these transformations. See Benecke at pg. 145. Because Benecke says nothing about the techniques used to place atoms and bonds in both two dimensions and three dimensions, we submit that Benecke is completely silent as to determining an arrangement of chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of an identified chemical structural symmetry.

Evidence that one having ordinary skill in the art and reading Benecke would conclude that MOLGEN+ merely considered symmetries to avoid duplications when generating all permutations of a list of elements is provided by the Declaration. Moreover, as set forth in the Declaration, one having skill in the art would not understand Benecke as disclosing or suggesting determining an arrangement of chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of an identified chemical structural symmetry or laying out the chemically symmetrically equivalent atoms and bonds in a two-dimensional pictorial representation of the chemical structure in accordance with the determined arrangement.

To restate simply, the use of chemical structural symmetry to remove redundant isomers during the process of generating constitutional isomers (*e.g.*, building connection tables) is not

equivalent to determining an arrangement of atoms and bonds to provide a visually symmetric expression of an identified chemical structural symmetry for use in laying out those atoms and bonds in a two-dimensional pictorial representation of a chemical structure. Thus, we submit claim 1 is not obvious over Helson in view of Benecke. Claims 9, 28, and 35 have comparable limitations to those of claim 1, and claims 13-27 and 29-34 depend from one of claim 1 or 28. Accordingly, we submit these claims are not obvious in view of the cited references for at least the same reasons given for claim 1.

Dependent claims 19-27 further limit the step of determining an arrangement of the chemically symmetrically equivalent atoms and bonds recited in claim 1. Regarding the dependent claims prior to this Amendment, the Examiner has taken official notice that a limited group of possible symmetries exist and a skilled artisan would employ them as appropriate. See Office Action at pg. 9. We traverse the taking of official notice and submit that the cited references are completely silent regarding determining an arrangement of atoms and bonds to provide a visually symmetric expression of an identified chemical structural symmetry for use in laying out those atoms and bonds in a two-dimensional pictorial representation of a chemical structure. Thus, the cited references also do not teach or suggest the specific claimed embodiments of this element of amended claim 1. Therefore, we submit that the specific techniques recited in the dependent claims are not common knowledge and respectfully request that the Examiner provide a specific reference that teaches or suggests the limitations found in dependent claims 19-27 to maintain the rejections of those claims.

In view of the above amendment, we submit the pending application is in condition for allowance.

Authorization to charge the fees for the three-month extension of time accompanies this Amendment. We believe no other fees are due with this response. However, if a fee is due, please charge our Deposit Account No. 08-0219, under Order No. 0103544.00131US2 from which the undersigned is authorized to draw.

Respectfully submitted,

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